

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 259 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.16e-01

Confidence level: 5.41e-01

Nearest Neighbors from the Training Set

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Chloranil

Measured: 209

Predicted: 259

Image not found

Chlorothalonil

Measured: 1820

Predicted: 1300

Image not found

Sulfone, methyl
pentafluorophenyl

Measured: 28.8

Predicted: 104

Image not found

2,3,4,5-Tetrachloroaniline

Measured: 1070

Predicted: 1470

Image not found

Etridiazole

Measured: 1000

Predicted: 82.5